

TUNNELING EFFECTS BETWEEN TORI IN DOUBLE WELLS¹

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Abstract: We consider tunneling between 2 symmetric potential wells for a 2-d Schrödinger operator, in the case of eigenvalues associated with quasi-modes supported on KAM or Birkhoff tori.

0. Introduction. We consider here tunneling between 2 symmetric potential wells for a 2-d Schrödinger operator $P = -h^2\Delta + V$ in the limit $h \rightarrow 0$, near some energy level $E_0 = 0$ close to the non degenerate minima of V .

Tunneling is a difficult problem that has exercised so far many subtle and ingenious strategies ; at least, computing tunneling rates involves various scenarios which depend on the details of the dynamics, ranging from integrable or quasi-integrable systems, to ergodic or chaotic ones (see [W], and [Cr] for a recent review.)

As a general rule, the energy shift (or splitting of eigenvalues) is related to the so called Agmon distance $S_0(E)$ between the wells, associated with the degenerate, conformal metric $ds^2 = (V - E)_+ dx^2$ that measures the life-span (instanton) of the particle in the classically forbidden region $V(x) \geq E$.

Much is known in the 1-d case, even for excited states, or in several dimensions for the lowest eigenvalues. For general wells, there is the following equivalence [Ma] : the corresponding normalized eigenfunctions are non exponentially small (i.e. for all $\varepsilon > 0$, larger, in local L^2 norm, than a constant times $e^{-\varepsilon/h}$, $0 < h \leq h_\varepsilon$,) where minimal geodesics, connecting the 2 wells, meet their boundary, if and only if the splitting is non exponentially small with respect to $e^{-S_0(E)/h}$.

We study the special case of splitting of eigenvalues associated with quasi-modes supported on KAM or Birkhoff tori ; our goal is to compute tunneling rates for a large family of such eigenvalues, which we shall call a *spectral tunnel series*.

1. Tori and quasi-modes. Let us consider for a moment the case of a single well around $U_0 = 0$ (so that we can ignore interaction with the other well,) and let $p_0(x, \xi) = \xi^2 + \lambda_1^2 x_1^2 + \lambda_2^2 x_2^2$ be the quadratic part of the (smooth) classical

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hamiltonian $p(x, \xi)$ near 0 (quadratic approximation). If the frequencies λ_j 's are rationally independent, then Birkhoff's theorem tells us that the orbits of p near the fixed point $(x, \xi) = 0$ with energy E are quasi-periodic, in the sense that they are confined within quasi-invariant tori (the Birkhoff tori,) over a time scale $\mathcal{O}(E^{-\infty})$. Whenever the system is non integrable, most of these tori, will be destroyed and replaced by chaotic regions ; however (under a suitable a diophantine condition on the frequencies,) the so-called KAM tori, whose collection form a Cantor set, eventually survive.

Such lagrangian (or possibly isotropic) integral manifolds Λ_ι^E support quasi-modes, whose energies are given by the Einstein-Brillouin-Keller (EBK) quantization rule : if $H(\iota) = 2\lambda_1\iota_1 + 2\lambda_2\iota_2 + \dots$ is the hamiltonian expressed (asymptotically) in terms of action-angle variables (ι, φ) , then the energies of the eigenstates are given to first order in h by :

$$(1) \quad E_\alpha(h) = H(\iota_\alpha), \quad \iota_\alpha = (\alpha + \frac{1}{4}\nu)h, \quad \alpha \in \mathbf{N}^2, \quad |\alpha|h \leq E_0$$

The vector $\nu = (2, \dots, 2)$ is Maslov index, counting the number of caustics met along an orbit, passing from sheet to sheet on the torus.

For Birkhoff tori associated with energies $Ch \leq E \leq h^\delta$, where $0 < \delta < 1$, EBK formula (1) can be corrected to all orders in h with an accuracy $\mathcal{O}(h^\infty)$ [Sj]. In case of KAM tori, and larger energies (in an interval independent of h ,) these expansions hold modulo $\mathcal{O}(e^{-1/Ch^{1/s}})$, for some $s > 1$ related to the diophantine condition on the ratio λ_1/λ_2 [Po]. Of course in that case, analyticity properties of the potential are required as in usual KAM procedures, which makes the analysis more subtle. But the geometry is the same.

We have seen that tunneling rates hinge upon decay of quasi-modes at the edge of the well $\partial U_E = \{V(x) = E\}$. They also depend on the decay near the caustics of Λ_ι^E , $\iota = \iota_\alpha$.

The caustics can be viewed as a rectangle shaped fold line delimiting the zone of pure oscillations of the quasi-modes, and touching the boundary of the wells at 4 vertices, the hyperbolic umbilic points (HU) points, section of the torus by the plane $\xi = 0$ in \mathbf{R}^4 . According to (1), the edges of this rectangle have a size $\iota_\alpha = (\alpha + \frac{1}{4}\nu)h$.

All tori Λ_ι^E continue analytically in the ξ variables. Over the classically forbidden region, analytic continuation amounts to parametrize the orbits with imaginary time. It is convenient to view Λ_ι^E as a multidimensional Riemann sheet structure, with a number of sheets corresponding to the choice of the sign of momentum, gluing along the caustics, and all intersecting at the HU's. Λ_ι^E is parametrized by a phase function $F_y^E(x)$, where $y \in \partial U_E$ denotes the umbilic and can be identified with ι . This phase is complex (reflecting the oscillations of the corresponding quasi-mode) on all but one sheet of Λ_ι^E , denoted by $\tilde{\Lambda}_\iota^E$, which lies over the classically forbidden region, and corresponds to a pure exponential decay of the quasi-mode (we exclude the sheet which gives exponential growth.)

In case of Birkhoff tori, we gave a complete asymptotic expansion of the quasi-mode in some region of the decaying zone [KaRo], close to, but at a finite

distance from the caustics. Similar expansions can be obtained closer to the caustics, in term of special functions of Airy type. Yet another expansion could be found in case of KAM tori.

2. Continuation of action integrals in the classically forbidden region. Another central geometric figure of the problem is the integral manifold of $q(x, \xi) = -p(x, i\xi)$ passing above ∂U_E , i.e.

$$\Lambda_\partial^E = \{\exp tH_q(\rho) : \rho \in \partial U_E \times 0, q(\rho) = -E, t \in \mathbf{R}\}$$

This is (locally) a smooth real lagrangian submanifold, of the form $\xi = \nabla d_E(x)$, $x \notin U_E$. where $d_E(x) = d_E(x, \partial U_E)$ is Agmon distance from x to ∂U_E . Actually, Λ_∂^E has the fibre bundle structure $\Lambda_\partial^E = \bigcup_{y \in \partial U_E} \gamma_y$. Here γ_y is the bicharacteristic of $q(x, \xi)$ at energy $-E$ issued from ∂U_E at the umbilic y , and $\gamma_y = \tilde{\Lambda}_\iota^E \cap \Lambda_\partial^E$.

Introducing appropriate coordinate charts of hyperbolic action-angle variables $(\iota', \varphi) \mapsto (\iota, \varphi')$ given by Birkhoff transformations, we can also view $F_y^E(x)$ as the action $\int_y^x \xi dx$ computed along some path keeping ι' constant, and varying φ . • Our first task is to continue $x \mapsto F_y^E(x)$ from $\tilde{\Lambda}_\iota^E$, keeping y and E fixed.

First we introduce some scaling factors. One difficulty throughout consists in the range of different scales. So let $\mu = \sqrt{E}$ be the characteristic size of the (euclidean) diameter of U_E .

Let $y = (y_1, y_2)$ be an umbilic, and assume that the torus Λ_ι^E is not “too flat” in a certain sense, or equivalently, that the rectangle shaped caustics is “not too far from being a square”. For x also close enough from γ_y , so that $F_y^E(x)$ is still real, we denote by $y(x)$ the unique point of ∂U_E such that $x \in \gamma_{y(x)}$. We have :

Proposition 1: $F_y^E(x)$ equals $d_E(x)$ precisely along the geodesic γ_y . Moreover

$$d_E(x) - F_y^E(x) \sim \frac{\partial^2}{\partial y_1^2} F_y^E(x)|_{x \in \gamma_y} (y_1 - y_1(x))^2 \sim -K(x, y) (y_1 - y_1(x))^2$$

where $K(x, y) \geq K_0 > 0$ whenever $\text{dist}(x, \partial U_E) \leq C\mu^{1/2}$. (here dist stands for the euclidean distance.) Denote by $\Gamma_y(x)$ the orthogonal projection of x onto γ_y .

Using a variant of Gauss Lemma (the geodesic flow is locally a radial isometry), Proposition 1 shows that there are smooth level surfaces $N_\mu(s) = \{d_E(x) = s\mu\}$, $s_1 \leq s \leq s_2$, $\text{dist}(N_\mu(s), \partial U_E) \sim \mu^{1/2}$, such that

$$(2) \quad d_E(x) - F_y^E(x) \sim -\frac{1}{\mu} (x - \Gamma_y(x))^2, \quad x \in N_\mu(s)$$

Using that eikonal equation is satisfied by both $d_E(x)$ and $F_y^E(x)$, estimate (2) continues in the large, all along γ_y , so far as γ_y does not reach any caustics. This holds in particular, if $\gamma = \Upsilon_E$ is a minimal d_E -geodesic between $N_\mu(s)$ and a fixed x_0 , somewhere in between the 2 wells. • Our second task is to compute action from continuation of energy surfaces, i.e. by varying E (and

ι' accordingly) but keeping x fixed. Let $(x, \xi(x)) = (x, \nabla_x d_E(x)) \in \Lambda_\partial^E$, and $(z', \zeta') = \kappa(x, \xi(x))$, where κ is a suitable canonical transform related to the mapping $(\iota', \varphi) \mapsto (\iota, \varphi')$, that preserves the boundary of the well : $\kappa(y, 0) = (y', 0)$.

In fact, we shall compute $d_E(x)$ in a $(\mu$ -independent) neighborhood ω of ∂U_E from Agmon distance $d_0(x)$ at energy 0, which is known to be a C^∞ function of x . We have : **Proposition 2:** For $x \in \omega$, $d_E(x) = d_0(x) + \sum_j \iota'_j \log \frac{z'_j}{y'_j} + \mathcal{O}(\mu^2)$.

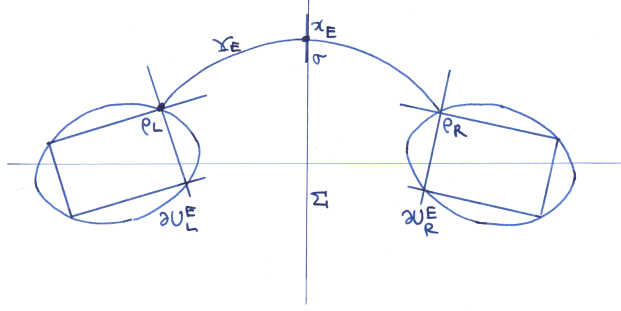
Typically, for $x \in \omega$, $\iota'_j \log \frac{z'_j}{y'_j}$ is comparable to $\mu^2 \log \mu$, so Proposition 2 gives the singularity of $d_E(x)$.

We look next how does $d_E(x, \partial\omega)$ depends on E in the large. For fixed x_0 away from ω , let Υ_E as above, be a minimal d_E -geodesic between $N = \partial\omega$ and x_0 , parametrized with arc-length. We can arrange so that N is a level surface for d_E . Using variations of geodesics as in [HeSj], we prove : **Proposition 3:** For all $\varepsilon > 0$, there is a $(\mu$ -independent) neighborhood Ω_E of $\Upsilon_E([0, 1 - \varepsilon])$, a μ^2 -neighborhood I_E of E , such that : (i) $(x, E') \mapsto d_{E'}(x, N) \in C^\infty(\Omega_E \times I_E)$. (ii) Ω_E is *starshaped*, in the following sense : $\forall (x, E') \in \Omega_E \times I_E, \exists ! d_{E'}$ -minimal geodesic joining N to x that stays in Ω_E . **3. The tunnel cycle.** We label

objects belonging the to left (resp. right) well with subscript L (resp. R). Extend $\Lambda_L = (\tilde{\Lambda}_L^E)_L$ along the bicharacteristic flow of q .

For a general, non integrable system, there is no reason for this extension coincides with $\Lambda_R = (\tilde{\Lambda}_L^E)_R$. However, we say that the pair $(\rho_L, \rho_R) \in \Lambda_L \times \Lambda_R$, are *in correspondance* along a bicharacteristic γ if Λ_L (or equivalently, because of symmetry, Λ_R) supports a quasi-mode, and $(\rho_L, \rho_R) \in \gamma \times \gamma$. We call the bicharacteristic γ a *tunnel cycle* if there is a pair (ρ_L, ρ_R) in correspondance along γ , with $(\rho_L, \rho_R) \in (\Lambda_\partial^E)_L \times (\Lambda_\partial^E)_R$. Then ρ_L and ρ_R are necessarily umbilics, and γ a geodesic between $U_L(E)$ and $U_R(E)$. A tunnel cycle will be called *minimal* if the geodesic γ is minimal, hence of lenght $d_E(U_L(E), U_R(E))$. Generically, bicharacteristics connecting pairs in correspondance and tunnel cycles are discrete sets. Moreover, pairs in correspondance, in case of Birkhoff tori, are only defined modulo $\mathcal{O}(E^\infty)$, since this is the case for $\tilde{\Lambda}_L^E$ and Λ_L^E . Tunnel cycles are exceptional, but as we shall see, there are many pairs in correspondance (belonging to different bicharacteristics) close to the umbilics. See [Gr] and [DoSh] for related notions.

a) The case of a minimal tunnel cycle. The picture is the following :



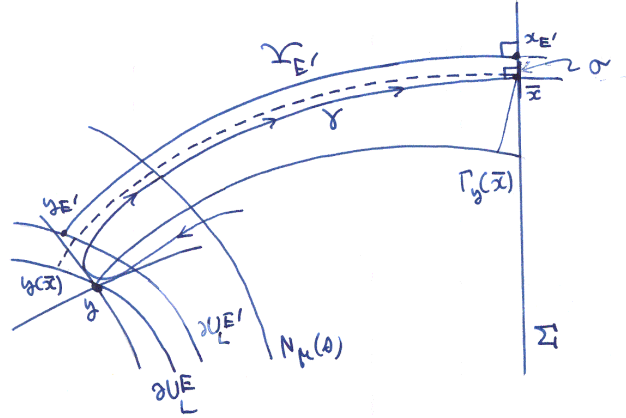
Let $u_L(x, E, h)$ and $u_R(x, E, h)$ be the quasi-modes associated with the umbilics ρ_L and ρ_R , continued beyond the symmetry axis Σ separating the 2 wells, in a neighborhood of the minimal geodesic Υ_E . Using Agmon estimates as in [HeSj], we can show that they approximate suitably the true eigenfunctions (provided a gap condition.) Assume for simplicity there is just one such minimal geodesic intersecting Σ at x_E . Since u_L and u_R are real near Σ , the eigenvalue splitting is given by the usual formula

$$(3) \quad E^+ - E^- = 4h^2 \int_{\sigma} u_L(0, x_2) \frac{\partial u_R}{\partial x_1}(0, x_2) dx_2 + \mathcal{O}(e^{-(S_0 + \varepsilon_0)/h})$$

where $\sigma \subset \Sigma$ is a neighborhood of x_E . Denote by $S_L - S_R^*$ the phase that comes up in (3), where S_L and S_R^* stand for suitable $F_y^E(x)$ as above. By the remark following Proposition 1, $S_L - S_R^*$ has a non degenerate critical point precisely at $x_E = \Upsilon_E \cap \sigma$. Moreover, the asymptotics of the quasi-modes near $U_L(E)$ given in [KaRo], propagate all along Υ_E , so the integral can be computed by standard stationary phase expansion around $x = x_E$. Since the amplitude of u_R (and u_L) is non vanishing, $E^+ - E^-$ is exactly of the order $e^{-S_0(E)/h}$.

b) The general case.

Given (ρ_L, ρ_R) in correspondance, we want to compare, for $x \in \Sigma$, the action $F_y^E(x)$ along the bicharacteristic connecting ρ_L and ρ_R with Agmon distance $d_{E'}(x)$ relative to a nearby energy value E' . For this, let $\Upsilon_{E'}$ be a minimal geodesic between $U_L(E')$ and $U_R(E')$, intersecting Σ at $x_{E'}$, the left and right components of $\partial U_{E'}$ at $y'_L = y_L(E')$ and $y'_R = y_R(E')$ respectively, and consider the *lattice of umbilics* carrying quasi-modes around such a point. At first approximation, umbilics are of the form $y = (\lambda_1^{-1} \sqrt{2\lambda_1 \iota_1}, \lambda_2^{-1} \sqrt{2\lambda_2 \iota_2})$, or by (1), $y = (\lambda_1^{-1} \sqrt{2h\lambda_1 \alpha_1}, \lambda_2^{-1} \sqrt{2h\lambda_2 \alpha_2})$, so the typical neighboring distance between umbilics is $h((\alpha_1 h)^{-1} + (\alpha_2 h)^{-1})^{1/2}$, which is greater than h/μ , but of the same order when tori are not “too flat”.



Let y be such an umbilic, and $\Lambda_L = (\tilde{\Lambda}_L^E)_R$ the corresponding Lagrangian manifold. It is easy to see that there is a bicharacteristic $\gamma \subset \Lambda_L \cap \Lambda_R$ (and points in correspondance) such that $S_L - S_R^*$ has a non degenerate critical point $\bar{x} \in \gamma \cap \Sigma$. We have :

$$(S_L - S_R^*) - S_0(E') = 2(F_y^E(\bar{x}) - d_E(\bar{x})) + 2(d_E(\bar{x}) - d_{E'}(\bar{x})) + 2(d_{E'}(\bar{x}) - d_{E'}(x_{E'}))$$

and combining Propositions 1-3 gives, under the above hypotheses, that $(S_L - S_R^*) - S_0(E') = o(1)$, as $h \rightarrow 0$, either in case of Birkhoff or KAM tori. To compute (3), one has also to know something about the amplitude, so we need to improve somewhat the expansions of [KaRo] when getting closer to the caustics.

References

- [Cr] S.C. Creagh. Tunneling in two dimensions. Proc. on "Tunneling in Complex systems" (INT 97-1) Seattle, April 30-May 30, 1997.
- [DoSh] S. Dobrokhotov, A. Shafarevich. Math. Phys. Anal. Geom. (2) p.141-177, 1999.
- [Gr] A. Grigis. Séminaire EDP, Exposé XXIII. Ecole Polytechnique. 1994-95.
- [HeSj] B. Helffer, J. Sjöstrand. Comm. Part. Diff. Eq. 9(4) p.337-408, 1984.
- [KaRo] N. Kaidi, M. Rouleux. Comm. Part. Diff. Eq., 27(9 and 10), p.1695-1750, 2002.
- [Ma] A. Martinez. Bull. Soc. Math. France 116 (2), p.199-219, 1988.
- [Po] G. Popov. Ann. H. Poincaré, Phys. Th. 1(2), p.223-248, 2000. Ann. H. Poincaré, Phys. Th. 1(2), p.249-279, 2000.
- [Sj] J. Sjöstrand. Asymptotic Analysis, 6, p.29-43, 1992.
- [Wi] M. Wilkinson. Physica 21D, p.341-354, 1986.